1«beta»-Acetoxyfuranoeudesm-4(15)-ene

Inchi: InChI=1S/C17H22O3/c1-10-5-6-16(20-12(3)18)17(4)8-15-13(7-14(10)17)11(2)9-19-15/h9
InchiKey: RVODLNSWAHTRAO-WIHSUSGWSA-N
Formula: C17H22O3
SMILES: C=C1CCC(OC(C)=O)C2(C)Cc3occ(C)c3CC12
Mol. weight [g/mol]: 274.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.77		Crippen Method
logp	3.591		Crippen Method
mcvol	218.220	ml/mol	McGowan Method
ripol	2663.00		NIST Webbook
ripol	2663.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R326046&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices

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